I U C L I D

Data Set

Existing Chemical	:	ID: 68425-16-1
CAS No.	:	68425-16-1
EINECS Name	:	Polysulfides, di-tert-nonyl
EC No.	:	270-336-2
Molecular Weight	:	414
Structural Formula	:	C9H19-S-S-S-S-S-C9H19
Molecular Formula	:	C18H38S5
Generic name	:	TPS 37

Producer related part

Company	:	Atofina
Creation date	:	09.07.2001

Substance related part

Company	:	Atofina
Creation date	:	09.07.2001
Status	:	
Memo	:	
Printing date	:	16.04.2004
Revision date	:	
Date of last update	:	16.04.2004
Number of pages	:	28
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS, temporary flag

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	
Name	:	Atofina
Contact person	:	
Date	:	
Street	:	4-8, cours Michelet La Défense 10
Town	:	95091 Paris La Défense Cedex
Country	:	France
Phone	:	+33 1 49 00 80 80
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

01.04.2004

Type	:	
Name	:	ATOFINA Chemicals Inc.
Contact person	:	
Date	:	
Street	:	2000 Market Street
Town	:	PA 19103 Philadelphia
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

01.04.2004

Type	:	
Name	:	Chevron Phillips Chemical Company LP
Contact person	:	
Date	:	
Street	:	10001 Six Pines Drive
Town	:	77380 The Woodlands, TX
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

16.04.2004

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :
Substance type : organic
Physical status : liquid
Purity :
Colour :
Odour :

30.07.2003

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Di-t-nonyl polysulfide

Source : Chevron Phillips Chemical Company LP The Woodlands, TX
08.12.2003

t-Nonyl polysulfide

Source : Chevron Phillips Chemical Company LP The Woodlands, TX
08.12.2003

tertiary-Nonyl polysulfide

Source : Chevron Phillips Chemical Company LP The Woodlands, TX
08.12.2003

TNPS, TPS 37

Source : ELF ATOCHEM ROTTERDAM B.V. VONDELINGENPLAAT/Rt
30.07.2003

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

Remark : Production process : Oxidation of nonyl mercaptan and mineral sulphur.
Two production plant.
Individual protective equipment (gloves, goggles).

Source : ELF ATOCHEM Paris la defense 10
30.07.2003

1.11 ADDITIONAL REMARKS

Remark : Transport : UN Number 3082
ADR/RID : Class 9 ; Item (letter) : 11°c ; Labels : 9 ;
H.I.Nr/ID Nr : 90/3082 ;
IMDG : Class 9 ; UN nr : 3082 ; Packaging group : III ;
Labels : MARINE POLLUTANT
IATA : Class : 9 ; Packaging group : III ; UN Nr(IATA) or
IDNr : 3082 ; Labels : 9.

Source : ELF ATOCHEM Paris la defense 10
30.07.2003

1.12 LAST LITERATURE SEARCH

Type of search : Internal and External
Chapters covered : 3, 4, 5
Date of search : 14.01.2004

Source : Atofina, Paris La Défense, France (JFR)
14.01.2004

Type of search : Internal and External
Chapters covered : 2
Date of search : 14.01.2004

Source : Atofina, Paris La Défense, France (JFR)
14.01.2004

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= 96.7 °C
Sublimation	:	
Method	:	other: calculated using EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di-tert nonyl polysulfide (CAS Number 68425-16-1)
Method	:	MPBPWIN (v 1.40) Selected Melting Point (Mean Value).
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

04.03.2004 (1)

Value	:	= -29 °C
Sublimation	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	TPS 37, DITERTIONONYL PENTASULFIDE, CAS: 68425-16-1
Source	:	Atofina, Paris-La Défense, France.
Reliability	:	(4) not assignable

08.01.2004 (2)

2.2 BOILING POINT

Value	:	= 350.6 °C at
Decomposition	:	
Method	:	other: calculated using EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di-tert nonyl polysulfide (CAS Number 68425-16-1)
Method	:	MPBPWIN (v 1.40) Boiling Point (Adapted Stein and Brown Method).
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

04.03.2004 (1)

Value	:	> 200 °C at
Decomposition	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	TPS 37, DITERTIONONYL PEBTASULFIDE, CAS no.68425-16-1
Source	:	Atofina, Paris-La Défense, France
Reliability	:	(4) not assignable

08.01.2004 (2)

2.3 DENSITY

Type	:	density
Value	:	= 1.024 g/cm³ at 20 °C
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	other TS
Source	:	Atofina, Paris-La Défense, France
Test substance	:	TPS 37, DITERTIONONYL PETASULFIDE, CAS no.68425-16-1
Reliability	:	(4) not assignable

08.01.2004 (2)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .0000343 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated): EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di-tert nonyl polysulfide (CAS Number 68425-16-1)
Method	:	EPIWIN Selected Vapor Pressure (Modified Grain Method). Vapor Pressure Estimations (25 deg C) using BP: 350.62 deg C (estimated) and MP: 96.7 deg C (estimated).
Remark	:	3.43E-5 hPa = 2.57E-5 mmHg.
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

04.03.2004 (1)

Value	:	< .03 hPa at 20 °C
Decomposition	:	
Method	:	other (calculated): no data
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	TPS 37, DITERTIONONYL PENTASULFIDE, CAS no.68425-16-1
Source	:	Atofina, Paris-La Défense, France
Reliability	:	(4) not assignable

08.01.2004 (2)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	
Log pow	:	= 9.14 at °C
pH value	:	

Method	:	other (calculated): EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Method	:	WSKOW v 1.40 -- estimated Log Kow.
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Test substance	:	di-tert nonyl polysulfide (CAS Number 68425-16-1)
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

04.03.2004 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	not soluble
Stable	:	
Deg. product	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	TPS 37, DITERTIONONYL PENTASULFIDE, CAS no.68425-16-1
Source	:	Atofina, Paris-La Défense, France
Reliability	:	(4) not assignable

08.01.2004 (2)

Solubility in	:	
Value	:	= .0001 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated using EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di-tert nonyl polysulfide (CAS Number 68425-16-1)
Method	:	Water Solubility calculated from Kow (WSKOW v 1.40).
Result	:	Calculated Water Solubility = 9.612E-5 mg/L
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

15.12.2003 (1)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 100 °C
Type	:	closed cup
Method	:	other: ASTM D93
Year	:	
GLP	:	no data
Test substance	:	other TS
Source	:	Atofina, Paris-La Défense, France
Test substance	:	TPS 37, DITERTIONONYL PENTASULFIDE, CAS no.68425-16-1
Reliability	:	(4) not assignable

08.01.2004 (2)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

Value	:	= 183.5 - mPa s (dynamic) at 20 °C
Result	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS
Source	:	Atofina, Paris-La Défense, France
Test substance	:	TPS 37, DITERTIONONYL PENTASULFIDE, CAS no.68425-16-1
Reliability	:	(4) not assignable

08.01.2004 (2)

Value	:	= 24 - 34 mPa s (dynamic) at 50 °C
Result	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS
Source	:	Atofina, Paris La-Défense, France.
Test substance	:	TPS 37, DITERTIONONYL PEBTASULFIDE, CAS no.68425-16-1
Reliability	:	(4) not assignable

08.01.2004 (2)

Value	:	= 4 - mPa s (dynamic) at 100 °C
Result	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS

Source	:	Atofina, Paris-La Défense, France
Test substance	:	TPS 37, DITERTIONONYL PEBTASULFIDE, CAS no.68425-16-1
Reliability	:	(4) not assignable

08.01.2004 (2)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	**other**
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di-tert nonyl polysulfide (CAS Number 68425-16-1)
Method	:	Calculated using EPIWIN v 3.10, AOP Program v 1.90.
Result	:	Overall OH Rate Constant = 473.0059 E-12 cm3/molecule-sec Half-Life = 0.023 Days (12-hr day; 1.5E6 OH/cm3) Half-Life = 16.281 Min
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

09.12.2003 (1)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	**fugacity model level III**
Media	:	other: air-water-soil-sediment
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: EPIWIN v 3.10
Year	:	2003
Test substance	:	di-tert nonyl polysulfide (CAS Number 68425-16-1)
Method	:	Used EPIWIN v 3.10. The following physical properties were used as the model input parameters: Chem Name: Di-tertiary-nonyl polysulfide Molecular Wt: 350.68 Henry's LC: 0.174 atm-m3/mole (Henrywin program) Vapor Press: 2.57E-5 mm Hg (Mpbpwin program)

Liquid VP: 0.000132 mm Hg (super-cooled)
Melting Pt: 96.7 deg C (Mpbpwin program)
Log Kow: 9.14 (Kowwin program)
Soil Koc: 5.66E+8 (calc by model)

Result : Results are provided in the following format:
Compartment / 100% to Air / 100% to Water / 100% to Soil / Equally to Each Compartment

Air / 75.0% / 3.95E-6% / 4.06E-6% / 0.00474%
Water / 0.0745% / 1.87% / 0.0021% / 1.28%
Soil / 21.0% / 5.13E-7% / 99.9% / 31.6%
Sediment / 3.91% / 98.1% / 0.11% / 67.1%

Air: half life = 0.5426 hr; emissions = 1000 kg/hr
Water: half life = 3600 hr; emissions = 1000 kg/hr
Soil: half life = 3600 hr; emissions = 1000 kg/hr
Sediment: half life = 1.44E+4 hr; emissions = 0 kg/hr

Persistence when distributed equally to each compartment = 5.47E+3 hr (Emissions [kg/hr] = 1000 to air, 1000 to water, 1000 to soil, and 0 to sediment).

Source : EPI Suite v 3.10.
Chevron Phillips Chemical Company LP The Woodlands, TX

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
10.12.2003 (1)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : **aerobic**
Inoculum : other: River water
Concentration : 800 mg/l related to Test substance
related to
Contact time : 28 day(s)
Degradation : < 0 (±) % after 28 day(s)
Result : under test conditions no biodegradation observed
Kinetic of testsubst. : 7 day(s) < 0 %
14 day(s) < 0 %
22 day(s) < 0 %
28 day(s) < 0 %
%
Control substance : Benzoic acid, sodium salt
Kinetic : 7 day(s) = 35.9 %
28 day(s) = 52.4 %
Deg. product : not measured
Method : Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
Year :
GLP : no data
Test substance :

Test substance : Test compound: TPS 37
Chemical name: di-t-nonyl polysulfide
CAS no.: 68425-16-1

Origine: Atochem
Batch: 6253
Total sulfur: no data

Test condition : INOCULUM/TEST ORGANISM
- Type of sludge: River water.
- Sampling site: Levallois
- Preparation of inoculum: Water was deducted from the river, decantated and filtred on a 0.22µm filter.The filter was rinsed with water and introduced for sowing flasks.
- Pretreatment:
- Initial cell concentration: 50 µl/l.

TEST SYSTEM
- Culturing apparatus: 300ml Erlenmeyers flasks.
- Number of culture flasks per concentration: 10.
- Aeration device: The solution was saturated with compressed air for 6 hours.
- Measuring equipment:Closed bottles.
- Closed vessels used: Yes.

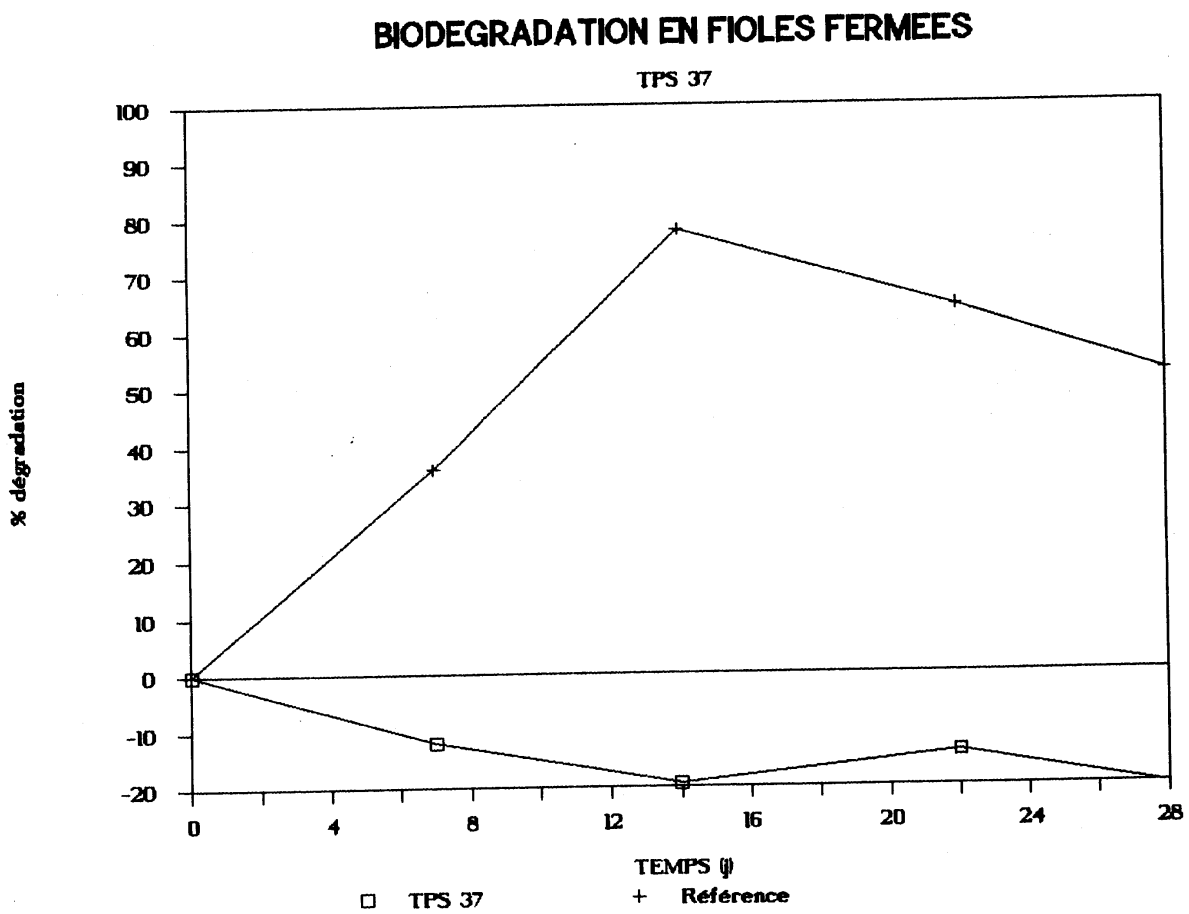
INITIAL TEST SUBSTANCE CONCENTRATION: 800 mg/l.
METHOD OF PREPARATION OF TEST SOLUTION:The substance was insoluble so it was introduced with acetone solvent which was evaporated before the test.
DURATION OF THE TEST: 28 days.
ANALYTICAL PARAMETER: The consumption of oxygen in the solution.The bacterial activity is evaluated by the consumption of dissolved O2, and the degradation follows from the difference between its consumption in flasks containing test substance and check flasks.
SAMPLING: 7, 14, 22, 28 days.
TEST CONDITIONS
- Composition of medium: For one litre of saturated water(with O2):

1- 1ml of solution a: KH_2PO_4 8.50g
K_2HPO_4 21.75g
Na_2HPO_4 33.40g
H_2O 1 litre.
2- 1ml of solution b: NH_4Cl 0.5g
H_2O 1 litre.
3- 1ml of solution c: $CaCl_2$ 27.5g
H_2O 1 litre.
4- 1ml of solution d: $MgSO_4,7H_2O$ 22.50 g
H_2O 1 litre.
5- 1ml of solution e: $FeCl_3$ 0.25g
E.D.T.A 0.40g
H_2O 1 litre.
6- water q.s.p 1000 ml.

- Additional substrate: No.
- Test temperature: 21+/-1°C.

INTERMEDIATES / DEGRADATION PRODUCTS: Not identified.
NITRATE/NITRITE MEASUREMENT: No.
CONTROLS:
REFERENCE SUBSTANCE: Benzoic acid,sodium salt.

Attached document : Courbe.bmp
Resultats.bmp



BIODEGRADATION EN FIOLES FERMEES

SUBSTANCE D'ESSAI: TPS 37
SUBSTANCE DE REFERENCE: BENZOATE DE SODIUM

ESSAI	FIOLE	TEMPS D'INCUBATION ,jours				
		0	7	14	22	28
		concentration oxygène (mg/l)				
BLANC	1	8,3	7,3	6,9	7,1	6,8
	2	8,4	7,3	6,9	7,0	6,6
	moyenne	8,35	7,30	6,90	7,05	6,70
ESSAI	1	8,1	7,6	7,5	7,5	7,5
	2	8,0	7,7	7,8	7,5	7,5
	moyenne	8,05	7,65	7,65	7,50	7,50
REFERENCE	1	8,3	6,8	4,4	4,8	5,0
	2	8,2	5,2	4,0	4,8	4,7
	moyenne	8,25	6,00	4,20	4,80	4,85

	Pourcentage de dégradation				
jours	0	7	14	22	28
ESSAI	0,0	-12,0	-19,4	-13,8	-20,3
REFERENCE	0,0	35,9	77,8	64,4	52,4

DThO (mg O2 / l)	
TPS 37	2,71
PhCOONa	1,67

Remark : Study Peer Reviewed.

Source	:	ATOFINA, PARIS-LA-DEFENSE, FRANCE.
Reliability	:	(1) valid without restriction
Flag	:	Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

16.04.2004 (3)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

BCF	:	75.66
Elimination	:	
Method	:	other: calculated using EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Method	:	Calculated using BCF Program (v 2.14).
Remark	:	Estimated Log BCF = 1.879 Estimated Koc = 2.797E+5 (using PCKOCWIN v 1.66)
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions

10.12.2003 (1)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	**static**
Species	:	Brachydanio rerio (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Limit test	:	yes
Analytical monitoring	:	yes
Method	:	Directive 92/69/EEC, C.1
Year	:	1992
GLP	:	yes
Test substance	:	

Test substance :

Test compound: TPS 37
Chemical name: di-t-nonyl polysulfide
CAS no.: 68425-16-1
Origine: Elf Atochem
Batch: no data
Total sulfur: 35.7% w/w

Test condition :

TEST ORGANISMS
- Strain: Brachydanio rerio.
- Supplier: Fish farming HB development, St Fargeux, FRANCE.
- Length: The animals were ranging from 3.1 to 3.3 cm.
- Acclimatisation: Animals were acclimated for 70 days in water (same quality, same temperature, same light... used in the test).

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Procedures: The test substance was dissolved in aqueous solution at 100 mg/l, agitated mechanically for 65 hours at 23°C.The substance not dissolved was filtered on Millipore GV 0.22µm.

DILUTION WATER:
According to EEC method C.1 92/69.
- 294 mg/l CaCl2, 2H2O
- 123.3 mg/l MgSO4, 7H2O
- 63.0 mg/l NaHCO3
- 5.5 mg/l KCl

TEST SYSTEM
- Nominal concentrations: 0.1 to 100 % vol.
- Number of replicates, fish per replicate: 5 fish per concentration
- Test temperature: 23.5+-1°C.
- Controled lighting : darkness 12/hours/24h)

The test was performed in 5 l glass crystallizing dishes closed with Altuglas plates.
2 vessels and 10 fishes were used per concentration.

TEST PARAMETER: Mortality or visible abnormalities.
MONITORING OF TEST SUBSTANCE CONCENTRATION: HPLC/MS.

Limit Test :
Saturated solution at 100 mg/l substance

- pH

Th	0	24	48	72	96
Saturated solution	8.60	7.80	7.81	7.91	7.76
Blank	7.86	7.83	7.80	7.82	7.79

- O2
Saturated 8.6 7.4 7.7 7.8 7.4
solution
Blank 8.5 7.8 7.8 7.6 7.7

Result : MORTALITY(%)

	24h	48h	72h	96h
Saturated solution	0	0	0	0
Blank	0	0	0	0

At the solubility limit of the substance in the test medium, no death of fishes was recorded at 96 hours.Thus, The substance was not toxic at the maximal concentration corresponding to the solubility limit in the test medium,
< 0.11 mg/l.

The study was performed in compliance with the following quality criteria : mortality in the control did not exceed 10% at the end of the test;concentration of dissolved oxygen in the test vessels remained above 60% of the air saturation value at the end of the test;pH did not vary by more than 1 unit.
Since it was not possible to determine the concentration of the substance at the limit of solubility (<0.11 mg/l), the validity criteria related to the test substance stability has not be checked.

Source : Atofina, Paris la Défense, France.
Reliability : (1) valid without restriction
Flag : Directive 67/548/EEC, Critical study for SIDS endpoint
16.04.2004 (4)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	**LD50**
Value	:	= 17781 - 21495 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	40
Vehicle	:	other: none
Doses	:	16000, 18000, 22000 and 24000 mg/kg
Method	:	other: comparable to OECD Guide-line 401
Year	:	
GLP	:	no
Test substance	:	

Test substance :

Test compound: TPS 37
Chemical name: di-t-nonyl polysulfide
CAS no.: 68425-16-1
Origine: Elf Aquitaine
Batch: no data
Total sulfur: no data

Test condition :

TEST ORGANISMS:
- Source: IFFA-CREDO
- Age: no data
- Weight at study initiation: 140-170 g
- Controls: no

ADMINISTRATION:
- Volume administered: 16 to 24 ml/kg of the undiluted test compound
- Post dose observation period: no

EXAMINATIONS: All animals were observed for mortality and signs of toxicity at 1, 2 and 6 hours post-dose and once daily thereafter for 14 consecutive days.
Individual body weights were recorded prior to treatment, on days 1, 2, 4, 7 and at termination.

STATISTICAL TEST: Mortality data were analyzed by the Litchfield and Wilcoxon's method

Result :

MORTALITY:

Dose mg/kg	Male	Female	Total
16000	2/5	0/5	2/10
18000	2/5	1/5	3/10
22000	1/5	5/5	6/10
24000	4/5	4/5	8/10

CLINICAL SIGNS:
- 16000 and 18000 mg/kg:
1 hour after treatment: lower spontaneous activity, apathy, prostration, piloerection, staggering step, slight closing of the palpebral slit .
6 hour after treatment: same symptoms.

Day 1 and 2: piloerection
Dqay 3: the surviving animals were normal.

-22000 et 24000 mg/kg:
Severe reduction of the spontaneous activity, apathy, prostration, staggering step. Loss of the reversal reflex in a female (24000 mg/kg).
6-24 hours after treatment: same clinical signs and diarrhea.
Day 2 : Piloerection in the surviving animals.
Day 3:
- 22000 mg/kg, recovery in the surviving animals.
- 24000 mg/kg distended abdomen.

Conclusion : The oral LD50 of TPS37 was 19550 (17781-21495) mg/kg.
Source : Atofina, Paris-la-Défense, France.
Reliability : (2) valid with restrictions
Flag : Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

26.02.2004 (5)

5.1.2 ACUTE INHALATION TOXICITY

Type : **LC50**
Value : > 15.5 mg/l
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals : 10
Vehicle : other: none
Doses : 15.5 mg/l
Exposure time : 4 hour(s)
Method : other: comparable to OECD Guide-line 403
Year :
GLP : no
Test substance :

Test substance : Test compound: TPS 37
Chemical name: di-t-nonyl polysulfide
CAS no.: 68425-16-1
Origine: Elf Aquitaine
Batch: no data
Total sulfur: no data

Test condition : TEST ORGANISMS:
- Source: IFFA-CREDO
- Age: no data
- Weight at study initiation: 150-200 g
- Number of animals: 5 males + 5 females
- Controls: no

ADMINISTRATION:
- Type of exposure: whole body
- Atmosphere generation: controlled fluid feed from a disposable plastic syringe driven by a syringe pump
- Concentration: nominal

EXAMINATIONS:
Duration of observation: 14 days
- Clinical signs: continuously during the exposure period, then daily until final sacrifice.
- Mortality: recorded once daily until the completion of the study.
- Body weight: measured on days 1, 3, 7 and 14.
- Necropsy: macroscopic examination of the main organs.

Result	:	CLINICAL SIGNS: . During exposure: From the very start of the exposure a very dense white fog settles in the chamber and limit the observation of the animals which remain huddled during the exposure. Only a reduction in the reaction to the noises from 45 min up to the absence of reaction can be highlighted. . After exposure: At the removal from the chamber the animals have wet fur and seek to flee. They present a slight irritation of the muzzle but recover a normal spontaneous activity after 15 mn. J 1: Closing of the palpebral slit, eyes cyanosed, polypnea and bronchial obstruction. J 2: one male died. J 4: all normal. NECROPSY: clear lungs
Conclusion	:	The inhalation exposur for 4 hours of 10 rats to a nominal concentration of 15.5 g/m3 TPS37 induced a mortality of 10%.
Source	:	Atofina, Paris-la-Défense, France.
Reliability	:	(2) valid with restrictions
Flag	:	Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

26.02.2004 (6)

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type	:	**LD50**
Value	:	= 3350 - 4375 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	30
Vehicle	:	other: none
Doses	:	3500, 4500 and 6000 mg/kg
Route of admin.	:	i.p.
Exposure time	:	
Method	:	other
Year	:	
GLP	:	no
Test substance	:	
Test substance	:	Test compound: TPS 37 Chemical name: di-t-nonyl polysulfide CAS no.: 68425-16-1 Origine: Elf Aquitaine Batch: no data Total sulfur: no data
Result	:	MORTALITY:

Dose (mg/kg)	Males	Females
3500	0/5	4/5
4500	2/5	5/5
6000	5/5	5/5

LD50: 3828 (3350-4375) mg/kg

CLINICAL SIGNS:
- 3 500 mg/kg:
1 hour after treatment: reduced spontaneous Activity, apathy, prostration, piloerection, slight closing of the palpebral slit
6 hours after treatment: same as above
D 2: Piloerection
D 3: Piloerection and eyes cyanosed in one female. Other survivors look normal

- 4 500 mg/kg:
Just after treatment: low spontaneous Activity, apathy, prostration, piloerection, closing of the palpebral slit
6 hours after treatment: moribund animals
D 1: Recovery of survivors
- 6 000 mg/kg: same as above, but more prononced, loss of the turning over reflexe.

Source : Atofina, Paris-la-Défense, France.
Reliability : (2) valid with restrictions
26.02.2004 (7)

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration : undiluted
Exposure : Occlusive
Exposure time : 24 hour(s)
Number of animals : 6
Vehicle :
PDII : 1.88
Result : slightly irritating
Classification : irritating
Method : other: JO RF 21/4/71, 5/6/73
Year : 1973
GLP : no
Test substance :

Test substance : Test compound: TPS 37
Chemical name: di-t-nonyl polysulfide
CAS no.: 68425-16-1
Origine: Elf Aquitaine
Batch: no data
Total sulfur: no data
Source : Atofina, Paris-la-Défense, France.
Reliability : (2) valid with restrictions
Flag : Material Safety Dataset, Directive 67/548/EEC
26.02.2004 (8)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration : undiluted
Dose : .1 ml
Exposure time : 24 hour(s)
Comment : not rinsed
Number of animals : 6
Vehicle :
Result : slightly irritating

Classification	:	not irritating
Method	:	other: JO RF 21/04/71 & 05/06/73
Year	:	1973
GLP	:	no
Test substance	:	
Test substance	:	Test compound: TPS 37 Chemical name: di-t-nonyl polysulfide CAS no.: 68425-16-1 Origine: Elf Aquitaine Batch: no data Total sulfur: no data
Source	:	Atofina, Paris-la-Défense, France.
Reliability	:	(2) valid with restrictions
Flag	:	Material Safety Dataset, Directive 67/548/EEC

26.02.2004 (8)

5.3 SENSITIZATION

Type	:	**Guinea pig maximization test**
Species	:	guinea pig
Concentration	:	1st: Induction 25 % intracutaneous 2nd: Induction 50 % occlusive epicutaneous 3rd: Challenge 1 % occlusive epicutaneous
Number of animals	:	30
Vehicle	:	
Result	:	not sensitizing
Classification	:	not sensitizing
Method	:	Directive 96/54/EC, B.6
Year	:	1996
GLP	:	yes
Test substance	:	other TS
Test substance	:	Test compound: TPS 37 LS Origine: Atofina SA Batch: 30-01-GF Total sulfur: 36.75% (w/w) Mercaptans: 1 ppm
Method	:	Thirty guinea pigs were allocated to two groups: a control group of five males and five females and a treated group of ten males and ten females. On day 1, three pairs of intradermal injections were performed in the interscapular region of all animals: · Freund's complete adjuvant (FCA) diluted at 50% (v/v) with 0.9% NaCl (both groups), · test item at the chosen concentration in the chosen vehicle (treated group) or vehicle alone (control group), · test item at the chosen concentration in a mixture FCA/0.9% NaCl (50/50, v/v) (treated group) or vehicle at the concentration of 50% (w/v) in a mixture FCA/0.9% NaCl (50/50, v/v) (control group). On day 8, the test item (treated group) or the vehicle (control group) was applied topically to the same test site, which was then covered by an occlusive dressing for 48 hours. On day 22, all animals of both groups were challenged by a cutaneous application of the test item to the right flank. The left flank served as control and received the vehicle only. The test item and vehicle were maintained under an occlusive dressing for 24 hours. Skin reactions were evaluated approximately 24 and 48 hours after

removal of the dressing.

Test item concentrations were as follows:

Induction (treated group)
· intradermal injections (day 1): TPS 37 LS at the concentration of 25% (w/w) in corn oil,
· topical application (day 8): TPS 37 LS at the concentration of 50% (w/w) in acetone.

Challenge (all groups)
· topical application (day 22): TPS 37 LS at the concentration of 1% (w/w) in acetone.

At the end of the study, animals were killed without examination of internal organs.
No skin samples were taken from the challenge application sites.

Result : No clinical signs and no deaths related to treatment were noted during the study.

No cutaneous reactions were observed after the challenge application.

Conclusion : According to the maximization method of Magnusson and Kligman, the test item TPS 37 LS (batch No. 30-01-GF) at the concentration of 1% does not induce delayed contact hypersensitivity in guinea pigs

Source : Atofina, Paris-la-Défense, France.
Reliability : (1) valid without restriction
Flag : Material Safety Dataset, Directive 67/548/EEC
26.02.2004 (9)

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type : **Salmonella typhimurium reverse mutation assay**
System of testing : Strains: TA 98, TA 100, TA 1535, TA 1537, TA 102
Test concentration : Experiment 1: 8, 40, 200, 1000 and 5000 µg/plate
Experiment 2: 4.883, 19531, 78.125, 312.5, 1250 and 5000 µg/plate
Cycotoxic concentr. : >= 1250 µg/plate
Metabolic activation : with and without
Result : negative
Method : Directive 84/449/EEC, B.14
Year : 1993
GLP : yes
Test substance :

Test substance : Test compound: TPS 37
Chemical name: di-t-nonyl polysulfide
CAS no.: 68425-16-1
Source: Elf Aquitaine Production
Batch: 47978
Sulfur content: 36.9%.

Test condition : SYSTEM OF TESTING
- 2 independent trials; in the 1st and 2nd trial without metabolic activation system (MA) the direct plate incorporation method was used; this method also used in the 1st trial with MA, in the 2nd trial with MA the preincubation method (1 h, 37°C). 3 plates per concentration
- Metabolic activation system (MA): S9 fraction from liver homogenates of rats induced with 500 mg/kg Aroclor 1254

- solvent: dimethylformamide
- Controls: . solvent control (with and without MA)
. Positives controls:
- Without S9
TA98: 2-nitrofluorene 5.0 µg/plate
TA100 and TA1535: Sodium azide 2.0 µg/plate
TA1537: 9-aminoacridine 50 µg/plate
TA102: glutaraldehyde 25 µg/plate
- With S9
TA98, TA100 and TA1535: 2-aminoanthracene 5.0 µg/plate
. sterility control checked during the test.
- Concentrations:
Experiment 1: 8, 40, 200, 1000 and 5000 µg/plate
Experiment 2: 4.883, 19531, 78.125, 312.5, 1250 and 5000 µg/plate
- Cytotoxicity: A preliminary toxicity test was performed to define the concentrations to be used for the mutagenicity study. TA100 exposed to 8-5000 µg/plate with and without MA

CRITERIA FOR EVALUATION
- negative and positive controls within the range of historical controls.
- positive: reproducible and significant dose related increase in revertants and/or reproducible doubling in the number of revertants compared with negative controls for one dose.

Result : Evidence of toxicity was observed at >=1250 µg/plate in only a few test strains. Precipitation of test agent was observed on all plates treated at concentrations >= 1000 µg/plate.

The mean numbers of revertant colonies on negative control plates all fell within acceptable ranges, and were significantly elevated by positive control treatments.

No TPS 37 treatment of any of the test strains produced an increase in revertant numbers sufficient to be considered as indicative of mutagenic activity.

Conclusion : TPS 37 did not induce mutation in five strains of Salmonella typhimurium (TA98, TA100, TA1535, TA1537 and TA102), when tested under the conditions employed for this study, which included treatments up to 5000 µg/plate, both in the absence and in the presence of a rat liver metabolic activation system (S-9).

Source : Atofina, Paris-la-Défense, France.
Reliability : (1) valid without restriction
Flag : Material Safety Dataset, Critical study for SIDS endpoint
26.02.2004 (10)

Type : **Chromosomal aberration test**
System of testing : Human Lymphocytes
Test concentration : 122.5, 175, 250 µg/ml
Cycotoxic concentr. : see freetext ME
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 473
Year : 1996
GLP : yes
Test substance :

Test substance : Test compound: TPS 37
Chemical name: di-t-nonyl polysulfide
CAS no.: 68425-16-1
Source: Elf Aquitaine Production
Batch: 47978
Sulfur content: 36.9%.

Method : TPS 37 was tested in an in vitro cytogenetics assay using duplicate human lymphocyte cultures from female donors in two independent experiments. The test article was dissolved in dimethyl formamide (used as vehicle control) and the highest dose level used, 250 µg/mL, was in excess of the solubility limit in culture medium.

In Experiment 1, treatment in the absence and presence of S-9 (rat liver post-mitochondrial fraction from Aroclor 1254 induced animals) was for 3 hours only followed by a 17 hour recovery period prior to harvest (3+17). The test article dose levels for chromosome analysis were selected by evaluating the effect of TPS 37 on mitotic index.
Chromosome aberrations were analysed at three consecutive dose levels (see below).
The highest concentration chosen for analysis, 250 µg/mL, induced no mitotic inhibition (reduction in mitotic index) in either the absence or presence of S-9.

S-9	Treatment+ recovery (hours)	Concentration (µg/ml)	Positive control
-	3+17	0, 122.5, 175, 250	NQO,2.5.µg/mL
+	3+17	0, 122.5, 175, 250	CPA, 25 µg/mL

In Experiment 2, treatment in the absence of S-9 was continuous for 20 hours. Treatment in the presence of S-9 (using S-9 prepared from animals induced with phenobarbitone and beta-naphthoflavone) was for 3 hours only followed by a 17 hour recovery period prior to harvest (3+17). Chromosome aberrations were analysed at three consecutive dose levels (see below). The highest concentration chosen for analysis was 250 µg/mL, which induced approximately 45 % and 11 % mitotic inhibition respectively.

S-9	Treatment+ recovery (hours)	Concentration (µg/ml)	Positive control
-	20+0	0, 122.5, 175 250	NQO, 2.5 µg/mL
+	3+17	0, 122.5, 175, 250	CPA, 30 µg/ml

Appropriate negative (solvent and untreated) control cultures were included in test system in both experiments under each treatment condition. The proportion of cell with structural aberrations in solvent cultures fell within historical solvent control ranges. 4-Nitroquinoline 1-oxide and cyclophosphamide were employed as positive control chemicals in the absence and presence of liver S-9 respectively. Cells receiving these were sampled in each experiment, 20 hours after the start of treatment; both compounds induced statistically significant increases in the proportion of cells with structural aberrations.

Result : Cultures treated with TPS 37 in the absence and presence of S-9 exhibited frequences of cells with structural aberrations (excluding gaps) which were similar to levels seen in concurrent negative controls. One culture treated with 122.5 µg/ml TPS 37 for 20 ours in the absence of S-9 exhibited frequencies of cells with structural aberrations which exceeded the historical negative control (normal) range. Insofar as the replicate culture at this dose exhibited frequencies within the normal range, the effect was considered to be of no biological relevance. All other test article treated cultures exhibited frequencies of cells with structural aberrations which fell within the normal range.

Conclusion : TPS 37 did not induce chromosome aberrations in cultured human peripheral blood lymphocytes when tested in excess of its limit of solubility in bo the absence and presence of S-9.

Source : Atofina, Paris-la-Défense, France.

Reliability : (1) valid without restriction

Flag : Material Safety Dataset, Critical study for SIDS endpoint
26.02.2004 (11)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

(1) United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation, 2000. EPI Suite v 3.10 (April, 2001).

(2) ATOFINA. Material safety data sheet. TPS37, DITERTIONONYL PENTASULFIDE, CAS: 68425-16-1, 17/01/2003.

(3) ATOCHEM. TPS 37, EVALUATION EN MILIEU AQUEUX DE LA BIODEGRADATION AEROBIE "ULTIME", ESSAI EN FIOLE FERMEE.CENTRE D'APPLICATION DE LEVALLOIS, RAPPORT n° 23737 LE 08/12/89.

(4) ELF ATOCHEM S.A., CAL, 2002.TPS 37. Toxicité aiguë vis-à-vis des poissons.Report N° 509/99//A.

(5) Elf Aquitaine, Ditertiononyl polysulfure-TPS 37, Essais de toxicité aiguë par voie orale et intrapéritonéale chez le rat. IFREB, study no. 911256, novembre 29, 1979.

(6) Elf Aquitaine, Ditertiononyl polysulfure-TPS 37, Essais de toxicité aïgue par voie repiratoire chez le rat. IFREB, study no. 911211, novembre 15, 1979.

(7) Elf Aquitaine, Ditertiononyl polysulfure-TPS 37, Essais de toxicité aïgue par voie orale et intrapéritonéale chez le rat. IFREB, study no. 911256, novembre 29, 1979.

(8) Elf Aquitaine Production, Ditertiononyl polysulfure (TPS 37), Tests de tolérance locale chez le lapin. IFREB, étude no. 911317, 9 novembre 1979.

(9) Atofina (2002) TPS 37 LS, SKIN SENSITIZATION TEST IN GUINEA PIGS (Maximization method of Magnusson and Kligman). CIT report no. 23043 TSG.

(10) Elf Aquitaine, TPS 37, Reverse mutation in five Histidine-requiring strains of Salmonella typhimurium. Covance Labatories Limited, study no. 154/35-D5140, may 1998.

(11) Elf Aquitaine, TPS 37, Induction of Chromosome Aberrations in Cultured Human Peripheral Blood Lymphocytes. Covance Labatories Limited, study no. 154/36-D5140, july 1998.

I U C L I D

Data Set

Existing Chemical	:	ID: 31565-23-8
CAS No.	:	31565-23-8
EINECS Name	:	di(tert-dodecyl) pentasulphide
Product name	:	TPS 32
EC No.	:	250-702-8
Molecular Formula	:	C24H50S5

Producer related part

Company	:	Atofina
Creation date	:	09.07.2001

Substance related part

Company	:	Atofina
Creation date	:	09.07.2001
Status	:	
Memo	:	chapters 3, 4 and 5 validated
Printing date	:	16.04.2004
Revision date	:	
Date of last update	:	16.04.2004
Number of pages	:	39
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS, temporary flag

1.0.1 APPLICANT AND COMPANY INFORMATION

Type :
Name : Atofina
Contact person :
Date :
Street : 4-8, cours Michelet La Défense 10
Town : 95091 Paris La Défense Cedex
Country : France
Phone :
Telefax :
Telex :
Cedex :
Email :
Homepage :

01.04.2004

Type :
Name : ATOFINA Chemicals Inc.
Contact person :
Date :
Street : 2000 Market Street
Town : PA 19103 Philadelphia
Country : United States
Phone :
Telefax :
Telex :
Cedex :
Email :
Homepage :

01.04.2004

Type :
Name : Chevron Phillips Chemical Company LP
Contact person :
Date :
Street : 10001 Six Pines Drive
Town : 77380 The Woodlands, TX
Country : United States
Phone :
Telefax :
Telex :
Cedex :
Email :
Homepage :

Source : Chevron Phillips Chemical Company LP The Woodlands, TX
04.03.2004

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

TPS 32 ;

Source : Elf Aquitaine Lacq
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

25.05.1994

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

Labelling	:	provisionally by manufacturer/importer
Specific limits	:	
Nota	:	, ,
R-Phrases	:	(53) May cause long-term adverse effects in the aquatic environment
S-Phrases	:	(61) Avoid release to the environment. Refer to special instructions/Safety data sets

04.03.2003

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

Type of limit : other: No occupational exposure limit available
Limit value :

Source : Atofina, Paris-la-Défense, France.
04.03.2003

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

Remark : Reaction of tert-Dodecyl mercaptan with sulfur (element) in presence of a catalyst.
H2S is eliminated by stripping.
Wastes to incinerators.
Hydrogen sulfide detectors.

Source : Elf Aquitaine Lacq
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
06.06.1994

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

Type of search : Internal and External
Chapters covered : 3, 4, 5
Date of search : 04.03.2003

Source : Atofina, Paris-la-Défense, France.
04.03.2003

Type of search : Internal and External
Chapters covered : 2
Date of search : 14.01.2004

Source : Atofina, Paris La Défense, France (JFR)
14.01.2004

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= 178.7 °C
Sublimation	:	
Method	:	other: calculated using EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di(tert-dodecyl) pentasulphide (CAS Number 31565-23-8)
Method	:	MPBPWIN (v 1.40) Selected Melting Point (Weighted Value)
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

04.03.2004 (1)

Value	:	< 0 °C
Sublimation	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Source	:	Atofina, Paris-La Défense, France.
Reliability	:	(4) not assignable

07.01.2004 (2)

Value	:	= -23 °C
Sublimation	:	
Method	:	other: no data
Year	:	
GLP	:	
Test substance	:	other TS
Test substance	:	TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
Source	:	Atofina, Paris-La Défense, France.
Reliability	:	(4) not assignable

07.01.2004 (3)

2.2 BOILING POINT

Value	:	= 463.6 °C at
Decomposition	:	
Method	:	other: calculated using EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di(tert-dodecyl) pentasulphide (CAS Number 31565-23-8)
Method	:	MPBPWIN (v 1.40) Boiling Point (Adapted Stein and Brown Method)
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

04.03.2004 (1)

Value : > 200 °C at 1013 hPa
Decomposition : yes
Method : other: no data
Year :
GLP : no data
Test substance : other TS

Test substance : TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Source : Atofina, Paris-La Défense, France.
Reliability : (4) not assignable
07.01.2004 (2)

Value : > 200 °C at
Decomposition :
Method : other: no data
Year :
GLP :
Test substance : other TS

Test substance : TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
Source : Atofina, Paris-La Défense, France.
Reliability : (4) not assignable
07.01.2004 (3)

2.3 DENSITY

Type :
Value : .95 g/cm³ at 20 °C
Method : other: no data
Year :
GLP :
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
Reliability : (4) not assignable
07.01.2004 (3)

Type : density
Value : = 1.01 g/cm³ at 20 °C
Method : other: no data
Year :
GLP : no data
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Reliability : (4) not assignable
07.01.2004 (2)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .0000000076 hPa at 25 °C

Decomposition	:	
Method	:	other (calculated): EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di(tert-dodecyl) pentasulphide (CAS Number 31565-23-8)
Method	:	MPBPWIN (v 1.40) Selected Vapor Pressure (Modified Grain Method)
Remark	:	7.6E-9 hPa = 5.7E-9 mmHg
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

04.03.2004 (1)

Value	:	< .01 hPa at 20 °C
Decomposition	:	
Method	:	other (calculated): no data
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Source	:	Atofina, Paris-La Défense, France.
Reliability	:	(4) not assignable

07.01.2004 (2)

Value	:	< .1 hPa at 20 °C
Decomposition	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS
Test substance	:	TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
Source	:	Atofina, Paris-La Défense, France.
Reliability	:	(4) not assignable

07.01.2004 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	
Log pow	:	= 11.86 at °C
pH value	:	
Method	:	other (calculated): EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Method	:	WSKOW v 1.40 Estimated Log Kow.
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Test substance	:	di(tert-dodecyl) pentasulphide (CAS Number 31565-23-8)
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

05.12.2003 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	
Value	:	< 0 mg/l at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	insoluble (< 0.1 mg/L)
Stable	:	
Deg. product	:	
Method	:	other: calculated using EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di(tert-dodecyl) pentasulphide (CAS Number 31565-23-8)
Method	:	WSKOW v 1.40 Water Solubility.
Result	:	Calculated Water Solubility = 5.368E-8 mg/L
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

04.03.2004 (1)

Solubility in	:	Water
Value	:	at 20 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	not soluble
Stable	:	
Test substance	:	TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Source	:	Atofina, Paris-La Défense, France.
Reliability	:	(4) not assignable

07.01.2004 (2)

Solubility in	:	Water
Value	:	at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	not soluble
Stable	:	
Deg. product	:	
Method	:	other: no data
Year	:	
GLP	:	
Test substance	:	other TS
Test substance	:	TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
Source	:	Atofina, Paris-La Défense, France.
Reliability	:	(4) not assignable

07.01.2004 (3)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : >= 121 °C
Type : closed cup
Method : other: ASTM D 93
Year :
GLP : no data
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Reliability : (4) not assignable
07.01.2004 (2)

Value : > 121 °C
Type : closed cup
Method : other: ASTM D 93
Year :
GLP :
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
Reliability : (4) not assignable
07.01.2004 (3)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

Result : flammable
Method :
Year :
GLP :
Test substance : other TS

Source : Elf Aquitaine Lacq
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Reliability : (4) not assignable
07.01.2004

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

Value : - 603 mPa s (dynamic) at 20 °C
Result :
Method :
Year :
GLP :
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Reliability : (4) not assignable
07.01.2004 (2)

Value : 54 - 74 mPa s (dynamic) at 50 °C
Result :
Method :
Year :
GLP :
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Reliability : (4) not assignable
07.01.2004 (2)

Value : - 7.9 mPa s (dynamic) at 100 °C
Result :
Method :
Year :
GLP :
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
07.01.2004 (2)

Value : - 207.7 mPa s (dynamic) at 20 °C
Result :
Method : other: no data
Year :
GLP :
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
Reliability : (4) not assignable
07.01.2004 (3)

Value : - 53 mPa s (dynamic) at 40 °C
Result :
Method : other: no data
Year :
GLP :
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
07.01.2004 (3)

Value : 22 - 34 mPa s (dynamic) at 50 °C

Result	:	
Method	:	other: no data
Year	:	
GLP	:	
Test substance	:	other TS
Source	:	Atofina, Paris-La Défense, France.
Test substance	:	TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
Reliability	:	(4) not assignable

07.01.2004 (3)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	**other**
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di(tert-dodecyl) pentasulphide (CAS Number 31565-23-8)
Method	:	AOP v 1.90: Hydroxyl Radicals.
Result	:	Overall OH Rate Constant = 683.5465 E-12 cm3/molecule-sec Half-Life = 0.016 Days (12-hr day; 1.5E6 OH/cm3) Half-Life = 11.266 Min
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

05.12.2003 (1)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	**fugacity model level III**
Media	:	other: air-water-soil-sediment
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: EPIWIN v 3.10
Year	:	2003
Method	:	Used EPIWIN v 3.10. The following physical properties were used as the model input parameters: Chem Name: Di-tertiary-dodecyl pentasulfide Molecular Wt: 498.97 Henry's LC: 2.27 atm-m3/mole (Henrywin program) Vapor Press: 5.7E-9 mm Hg (Mpbpwin program) Liquid Vapor Press: 1.89E-7 mm Hg (super-cooled) Melting Pt: 179 deg C (Mpbpwin program)

Log Kow: 11.9 (Kowwin program)
Soil Koc: 2.97E+11 (calc by model)

Result : Results are provided in the following format:
Compartment / 100% to Air / 100% to Water / 100% to Soil / Equally to Each Compartment

Air / 4.35% / 5.23E-9% / 6.99E-8% / 0.00323%
Water / 0.346% / 1.87% / 0.0021% / 1.27%
Soil / 77.1% / 3.67E-9% / 99.9% / 31.9%
Sediment / 18.2% / 98.1% / 0.11% / 66.9%

Air: half life = .3756 hr; emissions = 1000 kg/hr
Water: half life = 3600 hr; emissions = 1000 kg/hr
Soil: half life = 3600 hr; emissions = 1000 kg/hr
Sediment: half life = 1.44E+4 hr; emissions = 0 kg/hr

Persistence when distributed equally to each compartment = 5.5E+3 hr (Emissions (kg/hr) = 1000 to air, 1000 to water, 1000 to soil, and 0 to sediment)

Source : EPI Suite v 3.10.
Chevron Phillips Chemical Company LP The Woodlands, TX

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
08.12.2003 (1)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : **aerobic**
Inoculum : other: river water
Concentration : 800 mg/l related to Test substance
related to
Contact time : 28 day(s)
Degradation : = 0 (±) % after 28 day(s)
Result : under test conditions no biodegradation observed
Kinetic of testsubst. : 7 day(s) < 0 %
14 day(s) < 0 %
22 day(s) < 0 %
28 day(s) < 0 %
%
Control substance : Benzoic acid, sodium salt
Kinetic : 7 day(s) = 35.9 %
28 day(s) = 52.4 %
Deg. product : not measured
Method : Directive 84/449/EEC, C.3 "Biotic degradation - modified OECD screening test"
Year :
GLP : no data
Test substance : other TS

Test substance : Test compound: TPS 32
Chemical name: di-t-dodecyl polysulfide
CAS no.: 31565-23-8
Source: ATOCHEM

Batch: 6252
Sulfur content: no data

Test condition : INOCULUM/TEST ORGANISM
- Type of sludge: From river water
- Source: river water
- Sampling site: Levallois
- Preparation of inoculum: Water was deducted from the river, decantated and filtred on a 0.22µm filter.The filter was rinsed with water and introduced for sowing flasks.
- Initial cell concentration: 50µl/l

TEST SYSTEM
- Culturing apparatus: 300ml Erlenmeyer flask.
- Number of culture flasks per concentration: 10.
- Aeration device:the solution was saturated with compressed air for 6 hours.
- Closed vessels used: Yes.

INITIAL TEST SUBSTANCE CONCENTRATION: 800mg/l.
METHOD OF PREPARATION OF TEST SOLUTION: The substance was insoluble so it was introduced with acetone solvent which was evaporated before the test.

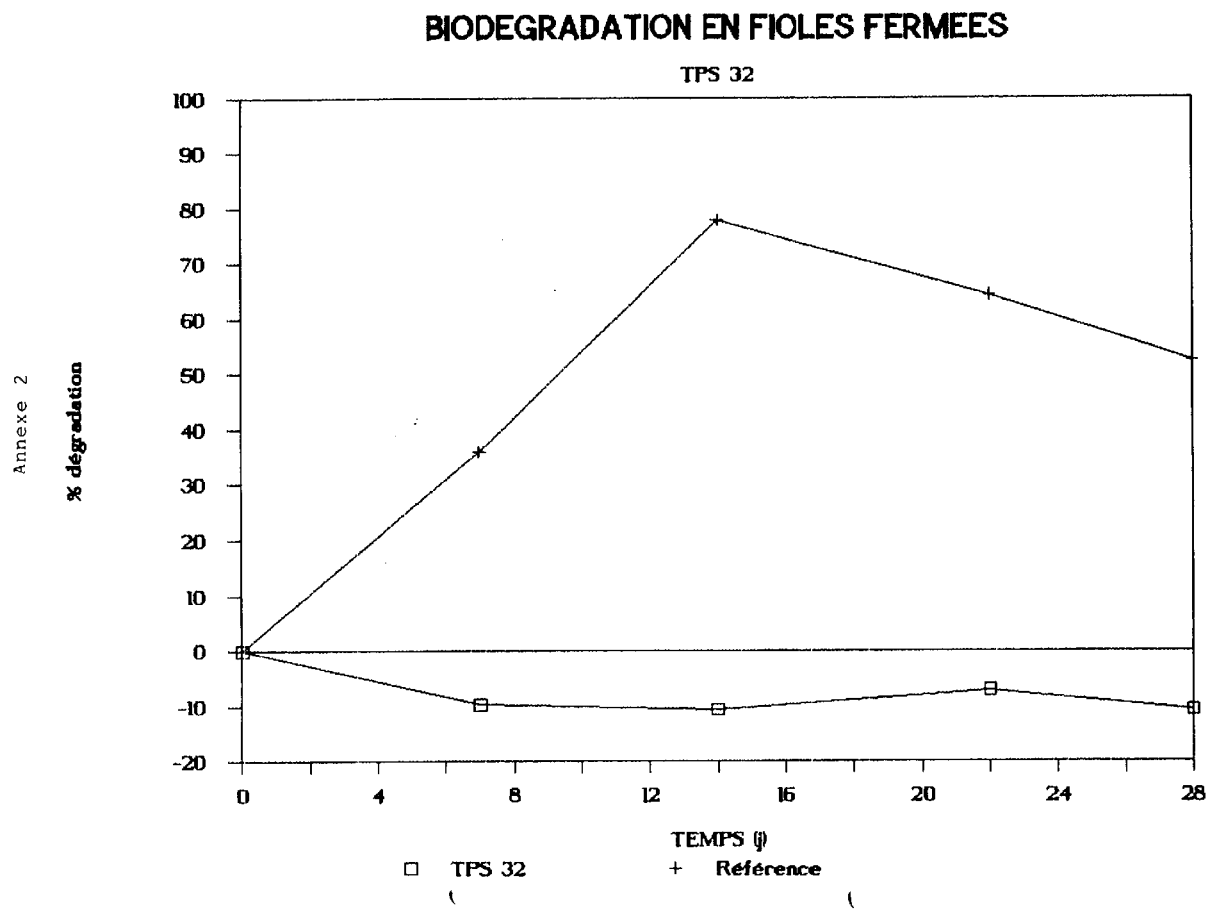
DURATION OF THE TEST: 28 days.

ANALYTICAL PARAMETER: The bacterial activity is evaluated by the consumption of dissolved O2, and the degradation follows from the difference between its consumption in flasks containing test substance and check flasks.
SAMPLING: 7, 14, 21, 28 days.

TEST CONDITIONS
- Composition of medium: For one litre of saturated water(with O2):
1- 1ml of solution a: KH2PO4 8.50g
K2HPO4 21.75g
Na2HPO4 33.40g
H2O 1 litre.
2- 1ml of solution b: NH4Cl 0.5g
H2O 1 litre.
3- 1ml of solution c: CaCl2 27.5g
H2O 1 litre.
4- 1ml of solution d: MgSO4,7H2O 22.50 g
H2O 1 litre.
5- 1ml of solution e: FeCl3 0.25g
E.D.T.A 0.40g
H2O 1 litre.
6- water q.s.p 1000 ml.

- Additional substrate: No.
- Test temperature: 21+/-1°C
INTERMEDIATES / DEGRADATION PRODUCTS: Not identified.
NITRATE/NITRITE MEASUREMENT: No.
REFERENCE SUBSTANCE: Benzoic acid,sodium salt.

Attached document : Courbe TPS 32.bmp



Conclusion	:	No degradation of TPS 32 was observed under the test conditions.
Source	:	ATOFINA, PARIS-LA-DEFENSE, FRANCE.
Reliability	:	(1) valid without restriction
Flag	:	Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

16.04.2004 (4)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

BCF	:	= 3.16
Elimination	:	
Method	:	other: calculated using EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di(tert-dodecyl) pentasulphide (CAS Number 31565-23-8)
Method	:	Calculated using BCF Program (v 2.14).
Remark	:	Estimated Log BCF = 0.500
		Estimated Koc = 1.9E+7 (using PCKOC Program v 1.66)
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions

15.12.2003 (1)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
Method	:	OECD Guide-line 202
Year	:	1984
GLP	:	yes
Test substance	:	other TS
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: ELF ATOCHEM Batch: 1209/98 Sulfur content: no data Appearance: yellow liquid or colourless Insoluble in water
Test condition	:	TEST ORGANISMS - Strain: Daphnia magna straus strain 5 or A. - Source/supplier: Breeding colony was realized in Elendt M7 medium in the laboratory, organisms were selected by sieving. - Breeding method: Not available. - Age: Less than 24 hours. - Feeding: Microscopic algae Raphidocelis subcapitata. - Pretreatment: No. - Feeding during test: No. - Control group: Yes. STOCK AND TEST SOLUTION AND THEIR PREPARATION - Preparation: Since TPS 32 is poorly soluble in water; a saturated solution was prepared by vigorously mixing: -100 mg of TPS 32 with dilution water during 23 hours at 20°C (preliminary test). - 2 mg of TPS 32 with dilution water during 68 hours at 20°C (definitive test). After this saturation period, the saturated solution was filtered with a HV 0.45 µm filter. - Vehicle, solvent: Ultrapure water. STABILITY OF THE TEST CHEMICAL SOLUTIONS: Not available, because the analytical method did not allow the determination of the test substance concentration. REFERENCE SUBSTANCE: Potassium dichromate. DILUTION WATER: was prepared in the laboratory using pure water and salts according to ISO 6341. For one litre: 25 ml of the below solutions 1- 11.76g CaCl2,2H2O/l ultrapure water. 2- 4.93g MgSO4,7H2O/l ultrapure water. 3- 2.59g NaHCO3/l ultrapure water. 4- 0.23g KCl/l ultrapure water.

- Aeration: aerated up until oxygen saturation.
- Ca/Mg ratio: 4.
- Na/K ratio: 10.

TEST SYSTEM
- Concentrations: 6.25, 12.5, 25, 50, 100 nominal concentration (% vol), forming a geometric progression with a factor of 2.
- Renewal of test solution: No.
- Exposure vessel type: 120 ml closed flasks with butyl rubber caps covered with PTFE.
- Number of replicates: 4.
- Number of individuals per replicate: 5 daphnids by replicate.
- Test temperature: 19-21°C.
- Dissolved oxygen: >2 mg/l.
- pH: 7.69-8.07.
- Adjustment of pH: No.
- Photoperiod: Incubation of test flasks in darkness.

DURATION OF THE TEST: 24 and 48 hours.
TEST PARAMETER: The percentage of daphnids immobilisation after 24 and 48 hours.
SAMPLING: 24, 48 hours.
MONITORING OF TEST SUBSTANCE CONCENTRATION: HPLC/MS.

Result : At the solubility limit of the test substance, no significative immobilization of the test organisms was recorded after 24 and 48 hours.

Thus the TPS 32 was not toxic for daphnia at the maximal exposure concentration corresponding to the solubility limit of the TPS 32 in the test medium.

The solubility limit of TPS 32 in the test medium was below the range of quantification (i.e.0.1 mg/l) and above the detection limit (i.e.0.02 mg/l) of the analytical method.

0.03 mg/l < Solubility limit <0.1 mg/l

- Nominal/measured concentrations: Attached document.
- Effect data (Immobilisation): Attached document.

RESULTS TEST WITH REFERENCE SUBSTANCE: The sensibility of the biologic reactive is controlled by a toxicity test with Potassium dichromate periodically, EC50/24h =1.1mg/l.

Attached document : Results TPS 32.bmp

6.1. Essai définitif

Le tableau ci-dessous présente les pourcentages d'immobilisation à 24h et 48h ainsi que les résultats des analyses chimiques réalisées par la méthode présentée en annexe 3.

Concentration				Immobilisation	
Nominale	Mesurée				
vol. solution. saturée (%)	Initiale (mg/l)	Finale (mg/l)	Final/Initial %	à 24 h (%)	à 48 h (%)
100	< LQ et > LD	< LQ et > LD	-	5	5
50	< LD	< LD	-	0	5
25	NA	NA	-	0	0
12,5	NA	NA	-	5	5
6,25	NA	NA	-	0	0

LQ : Limite de Quantification de la méthode d'analyse soit 0,1 mg/l.
LD : Limite de Détection de la méthode d'analyse soit 0,03 mg/l.
NA : concentration non analysée.

Remark : The method was applied with respect to its quality criteria:
- Immobilisation in the control did not exceed 10% at the end of the test.
- Concentration of dissolved oxygen in the test vessels remained above 2 mg/l at the end of the test.
- pH did not vary by more than 1 unit.

The solubility of the test substance in the test medium was below the limit of quantification of the analytical method. Therefore the stability of the substance during the assay has not been checked.

Source : ATOFINA, PARIS-LA-DEFENSE, FRANCE.
Reliability : (1) valid without restriction
Flag : Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

16.04.2004 (5)

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring : yes
Method : OECD Guide-line 202
Year : 1984
GLP : yes
Test substance : other TS

Test substance : Test compound: TPS 32
Chemical name: di-t-dodecyl polysulfide
CAS no.: 31565-23-8
Source: ELF ATOCHEM
Batch: 4352-96
Sulfur content: no data
Appearance: yellow liquid or colourless
Solubility: slightly soluble in water.

Test condition : TEST ORGANISMS
- Strain: Daphnia magna straus strain 5 or A.
- Source/supplier: Breeding colony was realized in Elendt M7 medium in the laboratory, organisms were selected by sieving.
- Breeding method: Not available.
- Age: Less than 24 hours.
- Feeding: Microscopic algae Raphidocelis subcapitata.
- Pretreatment: No.

- Feeding during test: No.
- Control group: Yes.

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Preparation: Since TPS is poorly soluble in water; 3 saturated solution were prepared by vigorously mixing:
-1, 10, 100 mg of TPS 32 with dilution water during 24 hours at 20°C. After this saturation period, the saturated solutions were centrifuged at 20°C, 2000g, during 20 mn.
- Vehicle, solvent: Ultrapure water.

STABILITY OF THE TEST CHEMICAL SOLUTIONS: Not available, because the analytical method did not allow the determination of the test substance concentration.

REFERENCE SUBSTANCE: Potassium dichromate.

DILUTION WATER: was prepared in the laboratory using pure water and salts according to ISO 6341.
For one litre: 25 ml of the below solutions
1- 11.76g $CaCl_2,2H_2O$/l ultrapure water.
2- 4.93g $MgSO_4,7H_2O$/l ultrapure water.
3- 2.59g $NaHCO_3$/l ultrapure water.
4- 0.23g KCl/l ultrapure water.
- Aeration: aerated up until oxygen saturation.
- Ca/Mg ratio: 4.
- Na/K ratio: 10.

TEST SYSTEM
- Concentrations: 1, 10, 100 mg/l.
- Renewal of test solution: No.
- Exposure vessel type: 120 ml closed flasks with butyl rubber caps covered with PTFE.
- Number of replicates: 4.
- Number of individuals per replicate: 5 daphnids by replicate.
- Test temperature: 19-21°C.
- Dissolved oxygen: >2 mg/l.
- pH: 8.07-8.14.
- Adjustment of pH: No.
- Photoperiod: Incubation of test flasks in darkness.

DURATION OF THE TEST: 24 and 48 hours.
TEST PARAMETER: The percentage of daphnids immobilisation after 24 and 48 hours.
SAMPLING: 24, 48 hours.

MONITORING OF TEST SUBSTANCE CONCENTRATION: HPLC/MS

Result **:** The percentage of immobilisation are presented in the following table for each of the 3 tested concentrations:

Mesured concentration		% of Immobilisation	
T0	T48	T0	T48
1.9	NA	5	100
0.31	NA	0	85
ND	NA	0	0

At the nominal concentration of 10mg/l, corresponding to a measured concentration of 0.31 mg/l, 85% of daphnids were immobilised.
Visual observations on the test solutions at nominal concentrations of 10 and 100 mg/l showed that the solubility limit of TPS 32 is probably lower than 0.31 mg/l.

Therefore the toxic effect of 85% may result from micro drops of non-solubilized test substance.

At the nominal concentration of 1mg/l, no toxicity was recorded and TPS 32 was not quantified since its concentration was below the detection limit of the analytical method i.e.0.04 mg/l.

Remark : In accordance with the study monitor, no analyse was performed at the end of the test.

Thus the quality criteria related to the stability of the substance all along the test duration has not been checked. Therefore, RESULTS OF THIS STUDY SHOULD BE INTERPRETED WITH CAUTION.

Source : ATOFINA, PARIS-LA-DEFENSE, FRANCE.
Reliability : (4) not assignable
Flag : Directive 67/548/EEC
16.04.2004 (6)

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 24 hour(s)
Unit : mg/l
EC0 : < .035
EC50 : = .449
EC100 : = 3.11
Analytical monitoring : no
Method : other: AFNOR NF T 90-301
Year :
GLP : no
Test substance : no data

Result : EC50,24h = 0.449 mg/l
EC50,24h corrected = 0.514 mg/l

EC100,24h = 3.11 mg/l
EC0,24h <0.035 mg/l

More informations:
At the concentration of 0.35 mg/l: pH = 7.89
At the concentration of 0.69 mg/l: pH = 7.80

Remark : The test was performed in presence of acetone as a solvent.
Source : Atofina, Paris-la-Défense, France.
Reliability : (4) not assignable
16.04.2004 (7)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : **other algae: Pseudokirchneriella Subcapitata**
Endpoint : growth rate
Exposure period : 72 hour(s)
Unit : mg/l
Limit test : no
Analytical monitoring : yes
Method : OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year : 1984
GLP : yes
Test substance : other TS

Test substance : Test compound: TPS 32
Chemical name: di-t-dodecyl polysulfide
CAS no.: 31565-23-8

Source: ELF ATOCHEM
Batch: 507/99
Sulfur content: no data
Appearance: yellow liquid or colourless
Insoluble in water

Method : - Analytical device:
pHmeter Mettler Toledo 345, Oxymeter WTW 538, Optical Microscope Zeiss RA34, Cytofluor 2350 microplate reader.

- Statistical test: Dunnett test.

Test condition : TEST ORGANISMS
- Strain: CCAP 278/4.
- Source/supplier: Culture Centre of Algae and Protozoa
- Method of cultivation: Parent cell suspensions were subcultured every week in 100 ml flasks, incubated at 23 ± 1°C, with alternative lighting (16h light / 8h darkness), under continuous aeration with filtrated Air (0.22µm).
- Pretreatment: 4 days before treatment, parent cultures are diluted (5 ml in 500 ml) to prepare 2 pre-cultures (one for sowing, the other for rescue).
- Controls: Quality of parent cultures was checked under a microscope to verify the absence of microorganisms or deformed cells.
- Initial cell concentration: 10000 cells/ml.

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Preparation: Since TPS is poorly soluble in water; a saturated solution was prepared by vigorously mixing 100 mg of TPS 32 with 1 litre of dilution water during 24 hours (this solution was agitated at 30°C for 3 hours and then at 23°C for 21 hours).
After this saturation period, droplets were observed on glass and in suspension in water. The saturated solution was filtered with a 0.22 µm filter.

- Vehicle, solvent: dilution water described below (in "Growth test medium chemistry") completed with NaHCO3 (0.3 g/l) and Hepes buffer state (6mM).

STABILITY OF THE TEST CHEMICAL SOLUTIONS: Not available, the concentration of TPS 32 in the saturated solution was not determined since it was assessed as below the detection limit of the analytical method.

REFERENCE SUBSTANCE:
Current method (C3, described in Directive 92/69/EEC) does not require a test with K2Cr2O7 as a quality criterion. However, the sensibility of the biologic reactive is controlled by a toxicity test with K2Cr2O7 every 2 months.

DILUTION WATER: was prepared by mixing ultrapure water with specific volume of the following solutions described below in Growth test medium.
-PH: 8 after equilibration with Air.
-Temperature: Dilution water must be preserved just for a few days at 23+/-2°C in darkness.

GROWTH TEST MEDIUM CHEMISTRY
Solution 1: Macronutriments
- NH4Cl : 15 mg/l
- MgCl2.6 H2O: 12 mg/l
- CaCl2.2 H2O: 18 mg/l
- MgSO4.7 H2O: 15 mg/l
- KH2PO4 : 1.6 mg/l

Solution 2: Fe-EDTA
- FeCl3.6 H2O: 0.08 mg/l

- Na2 EDTA.2 H2O: 0.1 mg/l

Solution 3: Oligoelements
- H3BO3 : 0.185 mg/l
- MnCl2.4 H2O : 0.415 mg/l
- ZnCl2 : 3x10-3 mg/l
- CoCl2.6 H2O : 1.5x10-3 mg/l
- CuCl2.2 H2O : 10-5 mg/l
- Na2MoO4.2 H2O : 7x10-3 mg/l

Solution 4: NaHCO3
- NaHCO3: 50 mg/l

TEST SYSTEM
- Test type: phytoculture chamber with rotating trays.
- Renewal of test solution: No.
- Exposure vessel type: 120 ml glass bottles stoppered with PTFE bungs and sealed with aluminium caps.
- Number of replicates per dose: 3.
- Concentrations: 9.39, 20.66, 45.45, 100 nominal concentration (% vol)forming a geometric progression with a factor of 2.2.
- Test temperature: 24 ± 1°C
- Intensity of irradiation: No data.
- Photoperiod: 16h light / 8h darkness.

pH and dissolved oxygen were measured at the beginning and the end of the test in the test solutions.

concentration nominale %vol	pH T0	pH T72h	Dissolved O2 T0	Dissolved O2 T72h
0	7.58	7.61	9.3	10
9.39	7.19	7.64	9.2	10.5
20.66	7.19	7.68	9.2	10.1
45.45	7.16	7.68	9.1	10.1
100	7.17	7.62	9.0	10.2

TEST PARAMETER: Inhibition of cellular multiplication.

MONITORING OF TEST SUBSTANCE CONCENTRATION: HPLC/MS.

Result : TPS 32 has a solubility limit of 0.080 mg/l in dilution water.

The results of this study show that NO INHIBITION OF GROWTH was observed after 72 hours of exposure to the saturated stock solution of TPS 32.

Growth curve: Attached document.

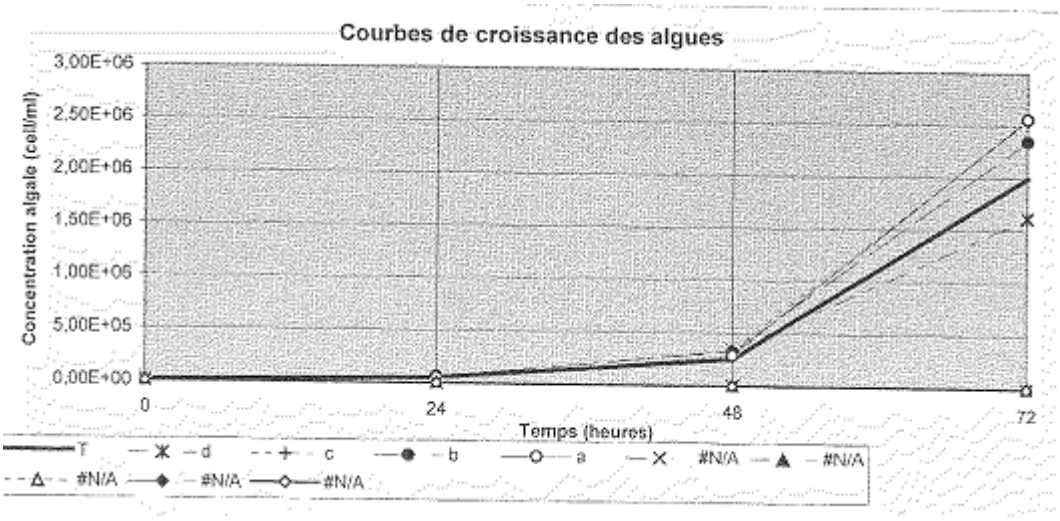
Cell density data: Attached document.
-A: Area under the curve
-µ: Growth rate

Inhibition percentages IA and Iµ: Attached document
IA: inhibition percentage based on Biomass.
Iµ: inhibition percentage based on Growth rate.

Attached document : TPS 32 A&µ.bmp
TPS 32 curve algae.bmp

Echantillon Référence	Concentration nominale (% Vol)	Concentration algale moyenne (cellules/ml) T0	T24h	T48h	T72h	$\bar{A}$	$\bar{\mu}$
T	0	10^4	$5,27\ 10^4$	$2,51\ 10^5$	$2,00\ 10^6$	$3,06\ 10^7$	0,0736
d	9,39	10^4	$5,47\ 10^4$	3,35 105	$1,62\ 10^6$	$2,82\ 10^7$	0,0707
c	20,66	10^4	$6,10\ 10^4$	$3,36\ 10^5$	$2,55\ 10^6$	$3,95\ 10^7$	0,0769
b	45,45	10^4	$6,10\ 10^4$	$3,29\ 10^5$	$2,35\ 10^6$	$3,70\ 10^7$	0,0758
a	100	10^4	$5,40\ 10^4$	$2,89\ 10^5$	$2,56\ 10^6$	$3,84\ 10^7$	0,0770

A: area under the curve
μ: growth rate



Remark : Study Peer Reviewed.
The appearance of the test solutions was visually checked at the beginning and the end of the test. Solutions were found to be clear. No precipitation was observed at the end of the test.

Microscopic observation confirmed that the algae appeared normal at the end of the test. The normal form of the unicellular algae is a crescent shaped cell with an average length of 5-10 µm.

QUALITY CRITERIA:
During the test the control pH varied by 0.52 units.

-The validity criterion of the study related to the growth of algae was respected: the increase in cell density (R) measured during the test was greater than a factor of 16 (R = 200).

-The validity criterion specific to C3 92/69EEC method and related to the test item stability during the test was not verified:
The concentration of TPS 32 in the saturated solution was not determined since it was assessed as below the detection limit of the analytical method.

Source : ATOFINA, PARIS-LA-DEFENSE, FRANCE.
Reliability : (1) valid without restriction
Flag : Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

16.04.2004 (8)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type :
Species : Pseudomonas putida (Bacteria)
Exposure period : 16 hour(s)

Unit	:	mg/l
Method	:	other: Norme ISO/TC 147/SC 5 WG 1(N111)
Year	:	
GLP	:	yes
Test substance	:	other TS
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: ATOCHEM Batch: 6252 Sulfur content: no data Appearance: yellow liquid Insoluble in water
Test condition	:	TEST ORGANISMS - Species: Pseudomonas Pituda MIGULA, Berlin 33/2. - Bacterial suspension: 50ml of solution I(described in the growth test medium)+ 125ml of solution II+ 50 ml of solution IV+ 18 g of Agar Gelose (microbiological use)+ Water q.s.p 1 litre. This mixture was sterilised at 120°C during 15 min. - Preculture medium: 25 ml solution I+25 ml solution III+50 ml solution IV. pH of this medium: 7.2+/-0.2. - Preparation: Inoculum was obtained from the preculture medium (less than 7 days), incubated during 7 hours for exponential phase growth. TEST SOLUTION: Since the TPS 32 was insoluble in water, 3 methods of introduction of TPS 32 were used: 1- TPS 32 was introduced directly in 100 ml of test medium by fractions from 10 mg to 1000mg. Flasks were placed under agitation during 16 hours at 21°C. 2- Formation of initial emulsion 5g/l of deionised water; by ultra sounds. Different dilutions of this emulsion were prepared until 1000mg/l. Flasks were placed under agitation during 16 hours at 21°C. 3- Dissolution of TPS 32 in DMF(diméthylformamide) forming an initial solution at 5g/l. In the different dilutions of this initial solution, the limit of DMF must be < 0.2% , above this limit the DMF have an inhibitory effect > 10% to bacteria. Flasks were placed under agitation during 16 hours at 21°C. REFERENCE SUBSTANCE: 3,5-dichlorophenol GROWTH TEST MEDIUM CHEMISTRY Solution I: NaNO3 10g K2HPO4 2.40g KH2PO4 1.20g Yeast 1g Water q.s.p 500ml Solution II: NaNO3 10g K2HPO4 2.40g KH2PO4 1.20g Water q.s.p 500ml Solution III: C6H12O6 solution C6H12O6,H2O 40g for biochemical and microbiological use Water q.s.p 500ml.

Solution IV:
MgSO4,7H2O 4g
Fe(III) citrate 0.01g, 19% Fe
Water q.s.p 1000ml

TEST SYSTEM
- Exposure vessel type: 250ml and 180 ml sterilised flasks.
- Test temperature: 21+/-1°C.
- Duration of the test: 16+/-1 hours.

TEST PARAMETER: Inhibition of cellular multiplication.
END POINT: Biomass, measured by Turbidity.

Result : It was not possible to detect an inhibitory effect of the substance towards Pseudomonas putida, in the 3 types of experiences.
The maximum concentration tested was 10 g/l.

*3,5 Dichlorophenol
CE50,16h = 18.3 mg/l.

Remark : Since the substance was insoluble in water, 3 types of experiences were realised:

- The test substance was directly put in culture medium.
- It was dispersed by ultra sounds.
- It was dissolved in dimethylformamide.

Study Peer Reviewed.

Source : ATOFINA, PARIS-LA-DEFENSE, FRANCE.
Reliability : (1) valid without restriction
Flag : Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

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4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	**LD0**
Value	:	> 12.5 ml/kg bw
Species	:	mouse
Strain	:	Swiss
Sex	:	male
Number of animals	:	40
Vehicle	:	other: undiluted
Doses	:	
Method	:	other
Year	:	1973
GLP	:	no
Test substance	:	
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: SNPA Batch: pure laboratory sample Sulfur content: no data
Test condition	:	The mortality was observed on a 7-day period. Clinical signs and body weight gain were not reported.
Source	:	Atofina, Paris-la-Défense, France.
Reliability	:	(2) valid with restrictions No additional details available.
Flag	:	Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

16.04.2004 (10)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	**LD0**
Value	:	>= 2000 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	20
Vehicle	:	other: none
Doses	:	
Method	:	OECD Guide-line 402 "Acute dermal Toxicity"
Year	:	1981
GLP	:	yes
Test substance	:	
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: SNEAP Batch: fabriquation Industrielle, no. 22463

		Sulfur content 30.53%
Result	:	CLINICAL EXAMINATIONS: No mortality and no behavioral anomaly were raised following the administration of the product and during the 14 following days. The local tolerance of the product was good: no cutaneous lesion (erythema or oedema) was raised at the site of application of the product during the observation period BODY WEIGHT GAIN: The body weight gain of the treated animals was not affected by the treatment. MACROSCOPIC EXAMINATIONS: No macroscopic abnormality was observed in the animals sacrificed at the end of the observation period.
Conclusion	:	The dermal LD0 of TPS 32 is higher than 2000 mg/kg.
Source	:	Atofina, Paris-la-Défense, France.
Reliability	:	(1) valid without restriction
Flag	:	Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

26.02.2004 (11)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	undiluted
Exposure	:	Semiocclusive
Exposure time	:	4 hour(s)
Number of animals	:	6
Vehicle	:	
PDII	:	
Result	:	slightly irritating
Classification	:	not irritating
Method	:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	:	1981
GLP	:	yes
Test substance	:	
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: SNEAP Batch: fabriquation Industrielle, no. 22463 Sulfur content 30.53%
Result	:	TPS 32 produced a slight erythema in one rabbit and a moderate erythema in 5 rabbits. A slight oedema was observed in 3 rabbits. Mean score (24+48+72 h) - Erythema : 1.72 - Oedema : 0.39
Source	:	Atofina, Paris-la-Défense, France.
Reliability	:	(1) valid without restriction
Flag	:	Material Safety Dataset, Directive 67/548/EEC

26.02.2004 (12)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	undiluted
Dose	:	.1 ml
Exposure time	:	24 hour(s)
Comment	:	not rinsed
Number of animals	:	6
Vehicle	:	
Result	:	slightly irritating
Classification	:	not irritating
Method	:	OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year	:	1981
GLP	:	yes
Test substance	:	
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: SNEAP Batch: fabriquation Industrielle, no. 22463 Sulfur content 30.53%
Result	:	TPS 32 incuced a slight chemosis and/or enanthema which persist for up to 72 hours in 2 animals. Slight iridal congestion was observed up to 48 hours in some animals. Mean scores (24 + 48 +72 h): - chemosis: 0.89 - Enanthema : 0.61 - Iris: 0.33 - Cornea: 0.00
Source	:	Atofina, Paris-la-Défense, France.
Reliability	:	(1) valid without restriction
Flag	:	Material Safety Dataset, Directive 67/548/EEC

26.02.2004 (13)

5.3 SENSITIZATION

Type	:	**Guinea pig maximization test**
Species	:	guinea pig
Concentration	:	1st: Induction 1 % intracutaneous 2nd: Induction undiluted occlusive epicutaneous 3rd: Challenge undiluted occlusive epicutaneous
Number of animals	:	30
Vehicle	:	
Result	:	ambiguous
Classification	:	not sensitizing
Method	:	OECD Guide-line 406 "Skin Sensitization"
Year	:	1986
GLP	:	yes
Test substance	:	
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: SNEAP Batch: fabriquation Industrielle, no. 22463 Sulfur content 30.53%
Method	:	. The applications corresponding to "the induction" were

carried out
- By intradermal route : injection of 2 x 0.1 ml
* on one hand, with the test article in a 1 % (W/V) solution in water for, injection ;
* on the other hand, with the 50/50 (V/V) mixing : test article in a 2 % solution (W/V) in water for injection + complete Freund's adjuvant at 50 % (V/V) in isotonic injectable solution, i.e. a final 1 % concentration of the sample to control.

Injection of the test article in a 1 % solution has provoked a weak to moderate irritation.

- By topical occlusive route for 48 hours, with the test article as supplied and at the dose level of 0.5 ml per animal.
This application having not provoked any weak to moderate irritation, a skin painting was carried out on Day 8, with 0.5 ml of Sodium Lauryl Sulfate at 10 % in Codex liquid paraffin.

- During the "challenge exposure", the topical occlusive application for 24 hours was carried out with the test article as supplied and at the dose level of 0.5 ml per guinea-pig (Maximum Non-Irritant Concentration : M.N.I.C.).

Result : From the macroscopic and histological results obtained under the experimental conditions, it may be concluded that the test article has provoked an aspecific reaction of
irritation of weak intensity in 4 out of the 20 treated guinea-pigs, this phenomenon can hide possible weak reactions of cutaneous sensitization, no characteristic cutaneous abnormality and different from the preliminary study was noted in the 10 control guinea-pigs.

Source : Atofina, Paris-la-Défense, France.
Reliability : (1) valid without restriction
Flag : Material Safety Dataset, Directive 67/548/EEC
26.02.2004 (14)

5.4 REPEATED DOSE TOXICITY

Type :
Species : rat
Sex : male/female
Strain : Sprague-Dawley
Route of admin. : gavage
Exposure period : 28 days
Frequency of treatm. : daily
Post exposure period : 14 days
Doses : 50, 250, 1000 mg/kg/d
Control group : yes, concurrent vehicle
NOAEL : = 1000 mg/kg bw
Method : Directive 84/449/EEC, B.7 "Sub-acute toxicity (oral)"
Year : 1992
GLP : yes
Test substance :

Test substance : Test compound: TPS 32
Chemical name: di-t-dodecyl polysulfide
CAS no.: 31565-23-8
Source: EAP

		Batch: 152319 (94_000858) Sulfur content 31.07%
Method	:	Two groups of six male and six female Sprague-Dawley rats received the TPS 32 daily by gavage at dose-levels of 50 or 250 mg/kg/day, and two groups of 12 males and 12 females was given 0 or 1000 mg/kg/day for four weeks. On completion of the four week treatment period, the first six surviving animals of each sex in the control and high dose groups were kept for a two week recovery period. Clinical signs and mortality were checked daily. Body weight and food comsumption were recorded once a week. Haematological and blood biochemical examinations and urinalysis were performed on week 5. At the end of the treatment period, all the surviving animals were killed and a macroscopic examination was performed. Designated organs were weighed and representative tissues specimen were submitted to a microscopic examination.
Result	:	No deaths related to the treatment occurred during the treatment period or the recovery period. Ptyalism was observed in all the animals of both sexes given 1000 mg/kg/day during the treatment period. Thereafter, during the recovery period, no clinical signs were observed. During the treatment and the recovery periods, the mean food consumption and body weight gain were similar between treated and control animals. No abnormalities of toxicological importance were noted among haematological and blood biochemical parameters, urinalysis, organ weights, macro- and microscopic examinations.
Conclusion	:	The No Observable Adverse Effect Level (NOAEL) was defined as 1000 mg/kg/day.
Source	:	Atofina, Paris-la-Défense, France.
Reliability	:	(1) valid without restriction
Flag	:	Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

26.02.2004 (15)

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	8 days
Frequency of treatm.	:	daily
Post exposure period	:	none
Doses	:	50, 250, 1250 and 2500 mg/kg
Control group	:	yes, concurrent vehicle
NOAEL	:	= 1250 mg/kg bw
LOAEL	:	2500 mg/kg bw
Method	:	other: range-finding study
Year	:	
GLP	:	no
Test substance	:	other TS
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: EAP Batch: 94_000670 Sulfur content 31.07%
Method	:	Four groups of 4 male and 4 female Sprague-Dawley rats received the TPS 32 daily by gavage at doses of 0, 50, 250, 1250 and 2500 mg/kg/day for 8 days. Clinical signs and mortality were checked twice daily. Food comsumption and

body weight were recorded twice a week. A complete macroscopic examination was performed on all animals killed at the end of the study. Adrenals, heart, kidneys, liver, spleen, thymus and gonades were weighed on all animals.

Result : No mortality occured during the treatment period. Ptyalism was observed in all the males given 1250 or 2500 mg/kg/day and in 2/4 or 3/4 females given 1250 or 2500 mg/kg/day, respectively. A slightly lower mean food consumption and body weight gain was observed in the males given 2500 mg/kg/d. Thickened and/or translucent wall of forestomach was noted for 3/4 females given 2500 mg/kg/day. No effect of treatment was observed on organ weights.

Source : Atofina, Paris-la-Défense, France.

Reliability : (2) valid with restrictions

26.02.2004 (16)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : **Salmonella typhimurium reverse mutation assay**
System of testing : Strains : TA 98, TA 100, TA 1535, TA 1537, TA 1538
Test concentration : 0, 5, 150, 500, 150, 5000 µg/plate
Cycotoxic concentr. : >= 5000 µg/plate
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471
Year : 1986
GLP : yes
Test substance :

Test substance : Test compound: TPS 32
Chemical name: di-t-dodecyl polysulfide
CAS no.: 68425-16-1
Source: SNEA(P)
Batch: 2246
Sulfur content: no data

Test condition : SYSTEM OF TESTING
- 2 independent trials; the direct plate incorporation method was used with and without métabolic activation (MA). 3 plates per concentration
- Metabolic activation system (MA): S9 fraction from liver homogenates of rats induced with 500 mg/kg Aroclor 1254
- solvent: ethanol
- Controls: . solvent control (with and without MA)
. Positives controls:
- Without S9
2-nitrofluorene: TA 98, 1.0 µg/plate; TA 1538, 2 µg/plate
ENNG: TA100, 3.0 µg/plate; TA 1535, 5 µg/plate
9-aminoacridine: TA1537, 80 µg/plate
- With S9
2-aminoanthracene: TA98, TA100 and TA1538, 0.5 µg/plate; TA 1535 and TA1535, 2 µg/plate
. sterility control checked during the test.
- Concentrations: 5, 150, 500, 150, 5000 µg/plate
- Cytotoxicity: A preliminary toxicity test was performed to define the concentrations to be used for the mutagenicity study. All strains exposed to 5-5000 µg/plate with and without MA

CRITERIA FOR EVALUATION
- negative and positive controls within the range of historical controls.
- positive: reproducible and significant dose related increase in revertants and/or reproducible doubling in the number of revertants compared with

negative controls for one dose.

Result : TPS-32 was not toxic towards the tester strains. Therefore 5000 µg/plate was chosen as the top dose level in the mutation tests.

No substantial increases in revertant colony numbers of any of the five tester strains were observed following treatment with TPS-32 at any dose level, either in the presence or absence of metabolic activation (S-9 mix).

Source : Atofina, Paris-la-Défense, France.
Reliability : (1) valid without restriction
Flag : Material Safety Dataset, Critical study for SIDS endpoint
26.02.2004 (17)

Type : **Chromosomal aberration test**
System of testing : human lymphocytes
Test concentration : 0, 300, 1000, 2500 µg/ml
Cycotoxic concentr. : > 2500 µg/ml (limit of solubility)
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 473
Year : 1983
GLP : yes
Test substance :

Test substance : Test compound: TPS 32
Chemical name: di-t-dodecyl polysulfide
CAS no.: 31565-23-8
Source: SNEA(P)
Batch D59B
Sulfur content 30.14%.

Method : The test substance was tested with and without a metabolic activation system, the S9 mix, prepared from a liver microsomal fraction (S9) of rats induced with Aroclor 1254.

The conditions of treatment were as follows, using 2 cultures/experimental point:
. without S9 mix: the cultures were incubated with the test or control substances which remained in the culture medium, until the appropriate harvest times*: 24 and 48 hours

. with S9 mix: the test or control substances remained in a culture medium containing 15% S9 mix (10% S9/S9 mix) for 2 hours. The cells were then centrifuged, the treatment medium removed, the cells resuspended in fresh culture medium. The cultures were then incubated until the appropriate harvest times*: 24 and 48 hours.

Two hours before harvesting, the cells were treated with a colcemid solution to block them at the metaphase-stage of mitosis. The chromosomal preparations were stained and screened microscopically for mitotic index and for aberrations: 200 well-spread metaphases per concentration were read, whenever possible.

The concentrations of TPS 32 for scoring were: 300, 1000 and 2500 µg/ml, 2500 µg/ml being the limit of solubility of the test substance in the culture medium.

Positive controls: Mitomycin C (0.2 µg/ml) without S9, Cyclophosphamide (50 µg/ml) with S9.

A reproducible and statistically significant increase in the aberrant cells

frequency for at least one of the tested concentrations is considered as a positive response.

* after the beginning of treatment

Result	:	For the test, the aberrant cells frequency in the negative and vehicle controls was within the range of our historical data (i.e. 0.5 ± 0.6%, gaps excluded). The aberrant cells frequency in the positive controls was significantly higher ($p < 0.001$) than that of the negative controls, indicating the sensitivity of the test system. The test substance did not induce any significant increase in the aberrant cells frequency, with or without S9 mix, for both of the 2 harvest times.
Conclusion	:	TPS 32 did not show clastogenic activity in this chromosomal aberration test performed in cultured human lymphocytes.
Source	:	Atofina, Paris-la-Défense, France.
Reliability	:	(1) valid without restriction
Flag	:	Material Safety Dataset, Critical study for SIDS endpoint

26.02.2004 (18)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	**rat**
Sex	:	female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	Gestation day 6 to 15.
Frequency of treatm.	:	daily
Duration of test	:	up to gestation day 20
Doses	:	50, 250 and 1000 mg/kg bw
Control group	:	yes, concurrent vehicle
NOAEL maternal tox.	:	= 1000 mg/kg bw
NOAEL teratogen.	:	= 1000 mg/kg bw
Method	:	OECD Guide-line 414 "Teratogenicity"
Year	:	1981
GLP	:	yes
Test substance	:	
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: EAP Batch: 96000424 Sulfur content 31.10%
Method	:	Three groups of 25 mated female rats received the TPS 32 by oral gavage at the dose levels of 0, 50, 250 or 1000 mg/kg/day, each day from day 6 to day 15 post-coitum inclusive.

Clinical signs (including evidence of abortion/resorption) and mortality were checked daily. Food consumption and body weight were recorded at designated intervals during pregnancy.
On day 20 post-coitum, females were killed. The gravid uterus was weighed and fetuses were removed by hysterectomy. Females were examined macroscopically. Litter parameters were recorded: number of corpora lutea, implantation sites, resorptions, dead and live fetuses. The live fetuses were weighed, sexed, submitted to an external examination and then to soft tissue or skeletal examinations.

Result : No clinical signs, no unscheduled deaths, no abortions or total resorption were observed in any group.
The food consumption and body weight gain of the pregnant females from all treated groups were similar to those of controls.
No treatment-related macroscopic findings were observed, in any group. The post-implantation loss was similar in the 0, 50 and 250 mg/kg-day groups. In the 1000 mg/kglday group, a slightly increased post-implantation loss (represented mainly by late resorptions, observed in one female) was observed: it could not be demonstrated that this single event was treatment-related.
No treatment-related effects were observed on the number of live fetuses per animal, the fetal body weight or the sex-ratio.
No treatment-related external anomalies or malformations were observed in any group. No treatment-related soft tissue malformations or anomalies were noted in any group. No treatment-related skeletal malformations, anomalies or variations were observed in any group.

Conclusion : The No Effect Level was defined as 1000 mg/kg/day in terms of maternotoxicity, embryo-fetotoxicity and teratogenic effects.

Source : Atofina, Paris-la-Défense, France.

Reliability : (1) valid without restriction

Flag : Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

26.02.2004 (19)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

(1) United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation, 2000. EPI Suite v 3.10 (April, 2001).

(2) Material Safety Data Sheet. TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0. ATOFINA, 25/02/2003.

(3) Material Safety Data Sheet. TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0. ATOFINA, 25/02/2003.

(4) ATOCHEM. TPS 32, 1989.Evaluation en milieu aqueux de la biodégradabilité aerobie "ultime", Essai en fiole fermée.Centre d'application de Levallois, n° rapport:23736.

(5) ELF ATOCHEM S.A. TPS 32. Toxicité Aiguë vis-à-vis des Daphnies. Centre d'application de Levallois, Etude N°: 1209/98/A, le 9/07/98.

(6) ELF ATOCHEM S.A. TPS 32, Toxicitié vis-à-vis des Daphnies. Centre d'application de Levallois, Etude N°: 4352/96/A, le 19/12/1997.

(7) ELF ATOCHEM, Centre d'Application de Levallois, 1988.
TPS 32/TPS 27/TPS 20/TPS 37. Détermination de l'inhibition de la mobilité de Daphnia magna selon la norme AFNOR NFT 90301.

(8) ELF ATOCHEM S.A. TPS 32. Inhibition de la Croissance des Algues. Centre d'application de Levallois, N° d'étude BPL: 507/99/A, le 06/03/2000.

(9) IRCHA, 1989. Etude B.7102. Determination d'un Effet Inhibiteur de la Multiplication Cellulaire Bactérienne pour le produit TPS 32.
(unpublished report).

(10) Rapport Laboratoire Henri Lauressergues, Etude de la Tolérance chez l'Animal de trois Polysulfures, 4 Juillet 1973.

(11) SNEA(P) Test pour l'Evaluation de la toxicité aiguë par administration cutanée unique (DL50), chez le rat. Rapport Hazleton-IFT N° 606358 du 13.06.1986.

(12) SNEA(P) Test pour l'évaluation de l'irritation primaire et de la corrosion cutanées aigues, chez le lapin. Hazleton-IFT N°606332 du 07.06.1986,

(13) SNEA(P) Test pour l'évaluation de l'irritation et de la corrosion oculaires, chez le lapin. Hazleton-IFT N°606332 du 07.06.1986.

(14) SNEA(P) Test pour l'évaluation du pouvoir sensibilisant chez le cobaye. Hazleton-IFT rapport N°606332 du 07.06.1986.

(15) Elf Aquitaine Production (1995) Four week toxicity study by oral route in rats followed by a two week recovery period with TPS 32, CIT Study No. 12602 TSR, 12 May 1995.

(16) Elf Aquitaine Production (1995) Preliminary 7-day toxicity study by oral route in rats, CIT Study No. 12601 TSR, 28 June 1995.

(17) SNEA(P) Ames Metabolic Activation Test to Assess the Potential Mutagenic Effect of TPS 32. Huntingdon Research Centre report no. ATO 20/86316, 3 april 1986.

(18) SNEA(P), TPS 32, In vitro Mammalian Cytogenetic test in cultures Human Lymphocytes. C.I.T. study no. 10309 MLH, january 5, 1994.

(19) Elf Aquitaine Production (1997) Study for effects on embryo-fetal development by oral route in rats with TPS 32. CIT Study No. 14706 RSR, 24 June 1997.